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ON THE COMPOSITION OF CIRCUMSTELLAR GRAINS

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ABSTRACT

On the basis of calculations of molecular equilibrium, it appears likely that circumstellar grains of oxygen-rich cool stars will be composed mainly of refractory silicates such as Mg_2SiO_4 and Al_2SiO_5. For carbon-rich stars the grains are mainly carbon, while for the transition stars silicon carbide predominates.

I. INTRODUCTION

As part of a program of theoretical studies of the atmospheric properties of cool stars, calculations of molecular equilibrium were performed that included condensates (solids and liquids) as well as gaseous compounds. These were full equilibrium calculations in the sense that all species, gaseous and condensate, were relaxed to their equilibrium abundances for a given temperature and total gas pressure. No attempt was made in these calculations to include the effects of nucleation or other time-dependent processes. The elements included in these calculations, and their relative abundances, are given in Table 1. Table 2 lists the compounds, gaseous and condensate, that were considered. The thermochemical data were taken from the JANAF *Thermochemical Tables* (1965), Tsuji (1964), Richardson and Jeffes (1949, 1952), Richardson (1953), Kelley (1962), Lord (1965), and Schick (1966)

Tsuji (1964) has published calculations of this type for one condensate (graphite), but, to the knowledge of this author, for many condensates and for conditions relevant to stellar atmospheres no calculations of this type have been published. (However, on the subject of circumstellar condensates, see Hoyle and Wickramasinghe 1962; Kamijo 1963, 1966; Donn *et al.* 1968; Wickramasinghe and Krishna Swamy 1968; and Fix 1968.) Our results, insofar as they overlap those of Tsuji (1964), are in essential agreement with his.

II. RESULTS

The bulk of the results of these calculations will be discussed in detail elsewhere. The intent of this Letter is to report some results of particular relevance to the infrared observations described elsewhere in this issue (Woolf and Ney 1969; Ney and Allen 1969; Knacke, Gaustad, Gillett, and Stein 1969; Stein and Gillett 1969), namely, the determination of the probable chemical composition of abundant condensates. These results are illustrated in Figure 1, which gives, for all the compounds included in the calculations, the temperature, T_c, at which significant condensation first occurs as a function of the oxygen-to-carbon abundance ratio (O/C). The total gas pressure of 50 dynes cm^{-2} used for this illustration is relevant to the upper atmosphere of red giants (cf. Auman 1967). For other pressures, T_c varies slightly, e.g., for Mg_2SiO_4 and O/C of 1.8, T_c goes from 1470° K for a gas pressure of 5×10^3 dynes cm^{-2} to 1200° K for a pressure of 0.5 dyne cm^{-2}. A similar variation occurs for the other compounds.

III. DISCUSSION

A discussion of the complex question of when solids can be expected to form in the atmospheres of cool stars is beyond the scope of this Letter. However, if such condensa-

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tion does take place, we can expect the composition of the condensates to be given essentially by Figure 1. Since not all possible relevant compounds and mixtures have been included in the calculations, because of the lack of thermochemical data, the exact composition of circumstellar grains may differ from that given here. For example, Mg_2SiO_4 may occur in the form of olivine, i.e., mixed with Fe_2SiO_4. However, abundance and chemical considerations suggest that modifications due to the inclusion of new compounds and mixtures will be of this type and will not change our qualitative results. In addition, preliminary considerations of the time-dependent nature of the formation of circumstellar grains (cf. Fix 1968) indicate no major changes in our results.

In summary, the results in Figure 1 and abundance considerations indicate that the important condensates for oxygen-rich stars will be refractory silicates such as Al_2SiO_5

TABLE 1

ASSUMED RELATIVE ABUNDANCES

Element	Abundance	Element	Abundance
H..........	1	S..........	1.5×10^{-5}
N..........	10^{-4}	Fe.........	3.75×10^{-6}
C...........	5×10^{-4} to 2×10^{-3}	Na........	2.0×10^{-6}
O...........	10^{-3}	Al.........	1.6×10^{-6}
Si..........	4.0×10^{-5}	Ca.........	1.4×10^{-6}
Mg.........	3.5×10^{-5}	Ni.........	8.0×10^{-7}

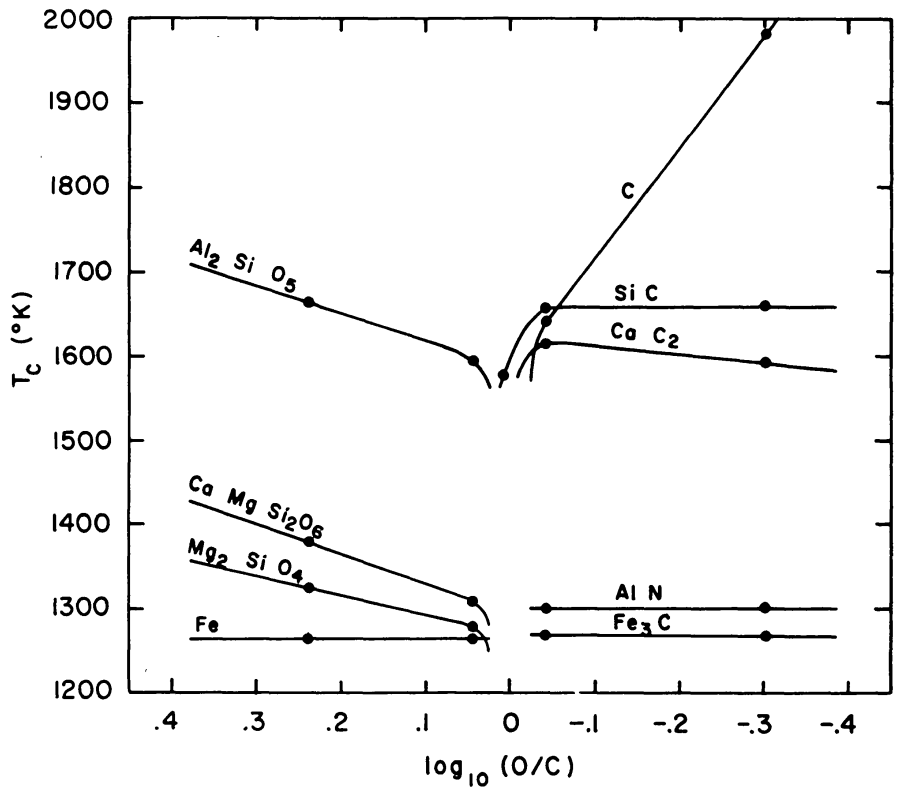

FIG. 1.—Temperature of the onset of condensation, T_c, as a function of $\log_{10}$ (O/C) for the compounds listed in Table 2 and for a total gas pressure of 50 dynes cm^{-2}. Dots represent actual computational results.

(with its relatively high T_c) and Mg_2SiO_4 (because of the relatively high abundance of magnesium). Carbon will be the dominant condensate for carbon-rich stars (high abundance and high T_c), while for the stars with approximately equal amounts of oxygen and carbon the most abundant condensate will be silicon carbide.

TABLE 2

COMPOUNDS CONSIDERED

Gaseous	Condensate	Gaseous	Condensate
H_2		FeO	Fe, FeO, Fe_2O_3, Fe_3O_4, Fe_2SiO_4, FeS, FeS_2, Fe_2C, Fe_3C
N_2			
C_2, C_3, C_4, C_5, CH, CH_2, CH_3, CH_4, C_2H, C_2H_2, CN, HCN	C	Na_2, NaH, NaO, NaOH, NaCN	Na, NaH, NaOH, NaCN, Na_2CO_3, NaO_2, Na_2O, Na_2O_2, Na_2SiO_3, $Na_2Si_2O_6$, Na_2S
O_2, OH, CO, CO_2, HCO, H_2CO, NO			
Si_2, Si_3, SiH, SiH_2, SiH_3, SiH_4, SiC, SiC_2, Si_2C, Si_2C_2, Si_2C_3, Si_3C_2, SiN SiO, SiO_2	Si, SiO_2, N_4Si_3, SiC	AlH, AlO, AlC, AlN, AlS, AlOH, $AlHO_2$, Al_2O, Al_2O_2	AlN, Al_2MgO_4, Al_2O_3, Al_2SiO_5, Al_4C_3, $AlNaSiO_4$, $AlNaSi_2O_6$, $AlNaSi_3O_8$, $FeAl_2O_4$
MgH, MgO, MgN, HMgO	MgO, $MgSiO_3$, Mg_2SiO_4, Mg_2Si, $CMgO_3$, C_2Mg, C_3Mg_2, H_2Mg, H_2MgO, Mg_3N_2	CaH, CaO	CaC_2, $CaSiO_3$, Ca_2SiO_4, Ca_3SiO_5, $Ca_3Si_2O_7$, CaO, CaS, $CaCO_3$, $Ca_2Al_2SiO_7$, $CaAl_2Si_2O_8$, $CaMgSi_2O_6$, $CaMgSiO_4$, Ca_2MgSiO_7, Ca_3MgSiO_8
S_2, SH, SO, SC, SN, SiS, MgS, SO_2, COS, CS_2	S_2Si, MgS, $MgSO_4$		
		NiO	Ni, NiO, Ni_3C

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